Defense Technical Information Center

Compilation Part Notice

ADP010898

TITLE: Small-Angle Multiple Scattering on a

Fractal System of Point Scatterers

DISTRIBUTION: Approved for public release, distribution unlimited

This paper is part of the following report:

TITLE: Paradigms of Complexity. Fractals and

Structures in the Sciences

To order the complete compilation report, use: ADA392358

The component part is provided here to allow users access to individually authored sections

of proceedings, annals, symposia, ect. However, the component should be considered within

the context of the overall compilation report and not as a stand-alone technical report.

The following component part numbers comprise the compilation report:

ADP010895 thru ADP010929

SMALL-ANGLE MULTIPLE SCATTERING ON A FRACTAL SYSTEM OF POINT SCATTERERS

V.V.UCHAIKIN

Ulyanovsk State University
Institute for Theoretical Physics
42 L.Tolstoy Str., 432700 Ulyanovsk, Russia
E-mail: uchaikin@sv.uven.ru

Multiple scattering of classical particles on a system of point scatterers distributed in space in a fractal fashion is considered in the small-angle approximation. The asymptotic regime of this process is described by a fractional differential equation generalizing the ordinary diffusion in the angle space equation. The solution of the problem is presented both in terms of stable distributions and in terms of Fox-functions. Main features of the obtained solutions are discussed.

1 Introduction

Small-angle x-ray and neutron scattering experiments are efficient tools for studying the structure of condensed matter. Measurements of the light or cosmic rays from distant sources play the same role in studying the large-scale structure of the Universe. From mathematical point of view, the problems belong to the class of inverse problems solved in terms of the multiple scattering theory.

The ordinary multiple scattering theory assumes that the random spatial distribution of scatterers is a homogeneous Poisson ensemble, i.e. different scatterers are placed independently of each other. That is just what guarantees the exponential character of the free path distribution and leads to the Boltzmann master equation. In the region of large depths and small angles the equation takes the form of the diffusion (in angle space) equation called the Fokker-Planck equation. Its solution is nothing but the two-dimensional (in angle space) Gauss distribution called also the Fermi distribution. However, above-mentioned assumption becomes invalid for fractal media characterized by long-range correlations of the power type.

One approach to solution of the problem is developed by S.Maleyev [1]. He has considered a medium with fractal pores distributed uniformly in space. As a result the superdiffusion behaviour of the angular distribution has been found. Another approach is developed in our previous work [2], where the fractal medium is considered as a set of identical point scatterers distributed in space in fractal manner by means of the Lévy flight procedure (see for details [3,4,5]). This model reveals the subdiffusion behaviour of the angle distribution.

The present work combines both of these ideas. We consider here a set of fractal clusters distributed in space in a fractal manner. As a result, we obtain a two-parametrical family of angular distributions. The family includes the Fermi distribution, the subdiffusion and superdiffusion distributions as particular cases. They obey fractional differential equations and are presented both in terms of stable distributions and in terms of Fox-functions.

2 Basic postulates of the small-angle scattering theory

Let a particle move from the origin of coordinates along the x-axis. After the scattering, the particle will be characterized by the vector angle $\vec{\Theta}$ of deviation from the initial direction $\vec{\Omega}_0$ of the motion

$$\vec{\Theta} = \vec{\Omega} - \vec{\Omega}_0.$$

The following postulates form the well-known basis of the small-angle approximation in the scattering theory.

i) The particle is on the x-axis during all its motion even though the (small) vector $\vec{\Theta}$ differs from zero.

ii) Vector $\vec{\Theta}$ stays constant between points of scatterings $X_1, X_1 + X_2, X_1 + X_2 + X_3, \ldots$ and undergoes random jumps $\vec{\Theta}_1, \vec{\Theta}_2, \vec{\Theta}_3, \ldots$ at these points, so

$$\vec{\Theta}(x) = \sum_{i=1}^{N(x)} \vec{\Theta}_i$$

where $N(x)$ is the random number of scatterings on the segment $[0, x]$.

iii) The random variables $X_1, X_2, X_3, \ldots$ are independent of each other and have the same distribution density $q(x)$.

iv) The random variables $\vec{\Theta}_1, \vec{\Theta}_2, \vec{\Theta}_3, \ldots$ are independent of each other and of $X_1, X_2, X_3, \ldots$ and identically distributed with the density $\sigma(\vec{\theta})$.

v) The distribution $\sigma(\vec{\theta})$ is concentrated in such a small region near zero that the vectors $\vec{\Theta}_i$ and $\vec{\Theta}(x)$ may be considered as two-dimensional vectors and integration with respect to $\vec{\theta}$ may be extended to the whole plane R^2.

On these assumptions, the angular distribution density $p(\vec{\theta}, x)$ of the particle passed the path x is given by the sum

$$p(\vec{\theta}, x) = \delta(\vec{\theta})Q(x) + \sigma(\vec{\theta}) \int_0^x Q(x - x')q(x')dx' +$$

$$\sigma * \sigma(\vec{\theta}) \int_0^x Q(x - x')q * q(x')dx' +$$

$$\sigma * \sigma * \sigma(\vec{\theta}) \int_0^x Q(x - x')q * q * q(x')dx' + \ldots \tag{1}$$

Here $*$ means convolution of distributions

$$q * q(x) \equiv \int_0^x q(x - x')q(x')dx',$$

$$\sigma * \sigma(\vec{\theta}) \equiv \int_{\mathrm{R}^2} \sigma(\vec{\theta} - \vec{\theta}')\sigma(\vec{\theta}')d\vec{\theta}',$$

and

$$Q(x) \equiv \int\limits_{x}^{\infty} q(x')dx'.$$

Represent (1) in the form

$$p(\vec{\theta}, x) = \int\limits_{0}^{x} Q(x - x')f(\vec{\theta}, x')dx'. \tag{2}$$

The function $f(\vec{\theta}, x)$ is the density of collisions and can be expanded in the collision number series

$$f(\vec{\theta}, x) = \delta(\vec{\theta})\delta(x) + \sigma(\vec{\theta})q(x) +$$

$$+\sigma * \sigma(\vec{\theta})q * q(x) + \sigma * \sigma * \sigma(\vec{\theta})q * q * q(x) + \ldots =$$

$$= \sum_{n=0}^{\infty} \sigma^{(n)}(\vec{\theta})q^{(n)}(x), \tag{3}$$

where

$$\sigma^{(0)}(\vec{\theta}) = \delta(\vec{\theta}), \quad \sigma^{(1)}(\vec{\theta}) = \sigma(\vec{\theta}), \quad \sigma^{(n)}(\vec{\theta}) = \underbrace{\sigma * \ldots \sigma(\vec{\theta})}_{n}, \quad n \geq 1$$

and so are $q^{(n)}(x)$. It is easy to see that the distribution (3) is a solution of the master equation

$$f(\vec{\theta}, x) = \delta(\vec{\theta})\delta(x) + \int\limits_{0}^{x} dx'q(x - x') \int\limits_{\mathbf{R}^2} d\vec{\theta}' \sigma(\vec{\theta} - \vec{\theta}')f(\vec{\theta}', x'). \tag{4}$$

Formula (2) together with master equation (4) gives a complete description of the problem.

3   The scattering theory for a homogeneous medium

The ordinary theory of multiple scattering appears as a result of the addition of two further postulates to those mentioned above:

vi) The mean square angle of a single scattering has a finite value

$$\langle \Theta^2 \rangle = \int\limits_{\mathbf{R}^2} \sigma(\vec{\theta})\theta^2 d\vec{\theta} = 2\pi \int\limits_{0}^{\infty} \sigma(\theta)\theta^3 d\theta < \infty.$$

vii) The random variables $X_1, X_1 + X_2, X_1 + X_2 + X_3, \ldots$ form the Poisson ensemble, i.e. the increments $X_1, X_2, X_3, \ldots$ are distributed according to the exponential law

$$q(x) = \mu e^{-\mu x}, \quad \mu > 0. \tag{5}$$

Inserting (5) into (2) and (4) we obtain two expressions

$$p(\vec{\theta}, x) = e^{-\mu x} \int_0^x e^{\mu x'} f(\vec{\theta}, x') dx',$$

$$f(\vec{\theta}, x) = \delta(\vec{\theta})\delta(x) + \int_{\mathrm{R}^2} d\vec{\theta'}\sigma(\vec{\theta} - \vec{\theta'})\mu e^{-\mu x} \int_0^x e^{\mu x'} f(\vec{\theta'}, x') dx'$$

which after simple transformations take a form of the integro-differential kinetic equation (the Boltzmann equation)

$$\frac{\partial p(\vec{\theta}, x)}{\partial x} = -\mu p(\vec{\theta}, x) + \mu \int_{\mathrm{R}^2} d\vec{\theta'}\sigma(\vec{\theta} - \vec{\theta'})p(\vec{\theta'}, x)$$

with the initial condition

$$p(\vec{\theta}, 0) = \delta(\vec{\theta}).$$

In the large x-asymptotics, the equation reduces to the ordinary diffusion equation

$$\frac{\partial p(\vec{\theta}, x)}{\partial x} = D\nabla_\theta^2 p(\vec{\theta}, x) \tag{6}$$

with $D = \mu\langle\Theta^2\rangle/2$. It is supposed here that $\sigma(\theta)$ is an axially symmetric function depending on $|\vec{\theta}| = \theta$.

4 The scattering theory for a fractal medium

A passage from a homogeneous medium to a fractal one is performed by the replacement of postulates vi) and vii) with the following:

vi)* The angular distribution of particles scattered on a single fractal cluster is characterized by the power law [1]

$$\int_{|\vec{\theta'}|>\theta} \sigma(\vec{\theta'})d\vec{\theta'} \sim A\theta^{-\alpha}, \quad \theta \to \infty, \quad 0 < \alpha < 2. \tag{7}$$

vii)* The free path distribution in a fractal path medium has a long power tail too [2]:

$$Q(x) \sim Bx^{-\beta}, \quad x \to \infty, \quad 0 < \beta < 1. \tag{8}$$

Note that the mean square angle in the first case and mean free path in the second one are infinite.

The information given by (7) and (8) is enough to find the asymptotic behaviour of the distribution $p(\theta, x)$ at large distances x. To do this we apply the Fourier-Laplace transform

$$p(\vec{k}, \lambda) = \int_{\mathrm{R}^2} d\vec{\theta} \int_0^\infty dx e^{i\vec{k}\vec{\theta} - \lambda x} p(\vec{\theta}, x),$$

where $\vec{k}$ is a two-dimensional vector and $\vec{k}\vec{\theta}$ is the scalar product. Formulas (2) and (4) take the following form:

$$p(\vec{k}, \lambda) = [1 - q(\lambda)]f(\vec{k}, \lambda)/\lambda,$$

$$f(\vec{k}, \lambda) = 1 + q(\lambda)\sigma(\vec{k})f(\vec{k}, \lambda).$$

Combining them we get

$$p(\vec{k}, \lambda) = \frac{1 - q(\lambda)}{\lambda[1 - q(\lambda)\sigma(\vec{k})]}.$$

This is the Montroll-Weiss result for random walk with trapping in a two-dimensional space [6] (see, also [7] and [8]).

According to the Tauberian theorem [9], the relations (7) and (8) determine behaviour of transforms $\sigma(\vec{k})$ and $q(\lambda)$ at small arguments:

$$1 - \sigma(\vec{k}) \sim ak^\alpha, \quad k \to 0, \quad a = \frac{2^{-\alpha}\Gamma(1 - \alpha/2)}{\Gamma(1 + \alpha/2)}A,$$

$$1 - q(\lambda) \sim b\lambda^\beta, \quad \lambda \to 0, \quad b = \Gamma(1 - \beta)B.$$

In their turn, these expressions make it possible to find the asymptotic form for $p(\vec{k}, \lambda)$:

$$p(\vec{k}, \lambda) \sim p_{as}(\vec{k}, \lambda) = \frac{\lambda^{\beta-1}}{\lambda^\beta + Ck^\alpha}, \quad \lambda \to 0, \quad k \to 0 \tag{9}$$

with $C = a/b$, whence

$$p_{as}(\vec{\theta}, x) = \frac{1}{(2\pi)^3 i} \int_L d\lambda \int_{R^2} d\vec{k} \frac{\lambda^{\beta-1}}{\lambda^\beta + Ck^\alpha} e^{-i\vec{k}\vec{\theta}+\lambda x} =$$

$$= (Cx^\beta)^{-2/\alpha} \Psi_2^{(\alpha,\beta)}(\vec{\theta}(Cx^\beta)^{-1/\alpha}) \tag{10}$$

where

$$\psi_2^{(\alpha,\beta)}(\vec{\theta}) = \frac{1}{(2\pi)^3 i} \int_{L'} d\lambda \int_{R^2} d\vec{k} \frac{\lambda^{\beta-1}}{\lambda^\beta + k^\alpha} e^{-i\vec{k}\vec{\theta}+\lambda}. \tag{11}$$

On the other hand, Eq. (9) rewritten in the form

$$\lambda^\beta p_{as}(\vec{k}, \lambda) = -Ck^\alpha p_{as}(\vec{k}, \lambda) + \lambda^{\beta-1},$$

can be considered as the Fourier-Laplace transform of the fractional differential equation. In terms used in the book [10] it has the form:

$$D_{x0+}^\beta p_{as}(\vec{\theta}, x) = -C(-\Delta_\theta)^{\alpha/2} p_{as}(\vec{\theta}, x) + \frac{x^{-\beta}}{\Gamma(1 - \beta)}\delta(x) \tag{12}$$

with the initial condition

$$p_{as}(\vec{\theta}, 0) = \delta(\vec{\theta}).$$

When $\alpha \to 2$ and $\beta \to 1$ the equation reduces to the ordinary diffusion equation (6) with $D = C$.

5 Results

The integral (11) giving the solution of the equation (12) via (10) may be represented in two forms [11]. The first of them is

$$\Psi_2^{(\alpha,\beta)}(\vec{\theta}) = \int\limits_0^\infty g_2^{(\alpha)}(\vec{\theta}x^{\beta/\alpha})g_1^{(\beta)}(x)x^{2\beta/\alpha}dx \qquad (13)$$

where $g_1^{(\beta)}(x)$ and $g_2^{(\alpha)}(\vec{\theta})$ are the one-dimensional one-sided stable density and the two-dimensional axially symmetrical stable density determined by their Laplace and Fourier transforms respectively:

$$\int\limits_0^\infty e^{-\lambda x}g_1^{(\beta)}(x)dx = e^{-\lambda^\beta}$$

and

$$\int\limits_{R^2} e^{i\vec{k}\vec{\theta}}g_2^{(\alpha)}(\vec{\theta})d\vec{\theta} = e^{-k^\alpha}.$$

Stable distributions are described in detail in [11,12].

The second form uses the H-functions – generalized hypergeometrical functions, also called the Fox functions [13],

$$H_{mn}^{pq}\left(z\left|\begin{array}{c}(a_1,\alpha_1)\dots(a_p,\alpha_p)\\(b_1,\beta_1)\dots(b_q,\beta_q)\end{array}\right|\right) = \sum_{j=1}^m\sum_{k=0}^\infty \frac{(-1)^k}{k!}c_{jk}z^{s_{jk}}/\beta_j,$$

where $m, n, p,$ and q are integer numbers such that $0 \le n \le p$ and $1 \le m \le q$; α_i and β_j are positive,

$$s_{jk} = (b_j + k)/\beta_j$$

$$c_{jk} = \frac{\prod\limits_{l=1,l\neq j}^m \Gamma(b_l - \beta_l s_{jk})\prod\limits_{l=1}^n \Gamma(1 - a_l + \alpha_l s_{jk})}{\prod\limits_{l=m+1}^q \Gamma(1 - b_l + \beta_l s_{jk})\prod\limits_{l=n+1}^p \Gamma(a_l - \alpha_l s_{jk})}.$$

In terms of H-function, the angular function $\Psi_2^{(\alpha,\beta)}(\vec{\theta})$ looks as follows

$$\Psi_2^{(\alpha,\beta)}(\vec{\theta}) = \frac{\beta}{8\pi}\left(\frac{2}{\theta}\right)^{2+\alpha} H_{32}^{12}\left(\left(\frac{2}{\theta}\right)^\beta\left|\begin{array}{c}(-1,1/\alpha)(-\alpha/2,\beta/2)(1-\alpha/2,1/2)\\(0,1/\alpha)(-1,1/\alpha)\end{array}\right.\right), \quad \alpha <$$

$$\Psi_2^{(\alpha,\beta)}(\vec{\theta}) = \frac{1}{\pi(\alpha\theta)^2}H_{23}^{21}\left(\frac{\theta}{2}\left|\begin{array}{c}(1,1/\alpha)(1,\beta/\alpha)\\(1,1/\alpha)(1,1/2)(1,1/2)\end{array}\right.\right), \quad 1 \le \alpha \le 2$$

When $\alpha = 2$ and $\beta = 1$

$$g_1^{(1)}(x) = \delta(x - 1),$$

$$g_1^{(2)}(\vec{\theta}) = \frac{1}{4\pi} \exp\left\{-\theta^2/4\right\} \tag{14}$$

and the density (13) reduces to the ordinary result for a homogeneous medium

$$p_{as}(\vec{\theta}, x) = \frac{1}{4\pi dx} \exp\left\{-\theta^2/(4Cx)\right\}$$

with the diffusivity C. This is the two-dimensional Gauss distribution with the mean square angle

$$\langle\theta^2\rangle = \int_{\mathbf{R}^2} p_{as}(\vec{\theta}, x)\theta^2 d\vec{\theta} = 4Cx, \tag{15}$$

describing a normal diffusion.

When $\alpha < 2$ and $\beta = 1$ we obtain

$$p_{as}(\vec{\theta}, x) = (Cx)^{-2/\alpha} g_2^{(\alpha)}(\vec{\theta}(Cx)^{-1/\alpha}).$$

The mean square angle is infinite now (due to the property of the density $g_2^{(\alpha)}$), but we may take

$$\delta\theta = (Cx)^{1/\alpha}$$

as the measure of the angular distribution width. This formula reveals a more rapid broadening of the angular distribution than in the normal case (15). We see here a superdiffusion regime considered in [1] (a more detailed consideration for N-dimensional space is performed in [14]).

When we have the opposite case, $\alpha = 2$ and $\beta < 1$, the mean square root of the scattering angle θ exists and is

$$\langle\theta^2\rangle^{1/2} = \left(\frac{4C}{\beta\Gamma(\beta)}\right)^{1/2} x^{\beta/2}, \quad \beta < 1.$$

This is a subdiffusion [15].

In the general case the rate of broadening the angular distribution is determined by the exponent β/α:

$$\delta\theta = C^{1/\alpha} x^{\beta/\alpha}.$$

Thus the multiple scattering reveals the subdiffusion asymptotic behaviour if $\beta/\alpha < 1/2$ and superdiffusion one if $\beta/\alpha > 1/2$. Both the regimes are covered by term "anomalous diffusion" (see [8,16] and references therein).

However, not only the rate of broadening the angular distribution changes by passing from homogeneous medium to fractal one: the very shape of the density changes too. Whereas $\Psi_2^{(2,1)}(\vec{\theta})$ is simply the two-dimensional Gaussian distribution, the densities $\Psi_2^{(\alpha,1)}(\vec{\theta})$, $\alpha < 2$, are two-dimensional symmetrical stable densities with characteristic exponent α. They have a dome-shaped form near zero with the maximum value

$$\Psi_2^{(\alpha,1)}(0) = \frac{\Gamma(1+2/\alpha)}{4\pi},$$

long tails of a power type

$$\Psi_2^{(\alpha,1)}(\vec{\theta}) \sim \left[\frac{\Gamma(1+\alpha/2)}{2\pi}\right]^2 \sin(\alpha\pi/2)\theta^{-\alpha-2}, \quad \theta \to \infty$$

and no moments of the order $\geq \alpha$ (see [10]). On the contrary, the densities $\Psi_2^{(2,\beta)}(\vec{\theta})$, $\beta < 1$, diverge logarithmically at zero

$$\Psi_2^{(2,\beta)}(\vec{\theta}) \sim \frac{|\ln\theta|}{2\pi\Gamma(1-\beta)}, \quad \theta \to 0.$$

rapidly falling tails

$$\Psi_2^{(2,\beta)}(\vec{\theta}) \sim \frac{\beta^{(3\beta/2-1)/(2-\beta)}}{4\pi\sqrt{2-\beta}} \times$$

$$\times (\theta/2)^{-2(1-\beta)/(2-\beta)} \exp\left\{-(2-\beta)\beta^{\beta/(2-\beta)}(\theta/2)^{2/(2-\beta)}\right\}, \quad \theta \to \infty \qquad (16)$$

and finite moments of all positive orders

$$\int_{\mathbf{R}^2} \theta^{2n}\Psi_2^{(2,\beta)}(\vec{\theta})d\vec{\theta} = 4^n \frac{[\Gamma(n+1)]^2}{\Gamma(\beta+1)}.$$

Note that (16) reduces to (14) when $\beta \to 1$.

In the case $\alpha = 1$, $\beta = 1/2$, the density $\Psi_2(\vec{\theta})$ is expressed in terms of the incomplete gamma function:

$$\Psi_2^{(1,1/2)}(\vec{\theta}) = (4\pi)^{-3/2}e^{\theta^2/4}\Gamma(-1/2, \theta^2/4).$$

Acknowledgments

References

1. S.V.Maleyev, *Phys. Rev. B*, **52**, 13163 (1995).
2. V.V. Uchaikin, D.A. Korobko, *Techn. Physics Letters*, **25**, 435 (1999).
3. V.V.Uchaikin, G.G.Gusarov, *J.Math.Phys.*, **38**, 2453 (1997).
4. V.Uchaikin, I.Gismjatov, G.Gusarov, V.Svetukhin, *Intern. J. Bif. and Chaos*, **8**, 977 (1998).
5. V.V.Uchaikin, G.G.Gusarov, D.A.Korobko, *Journ. Math. Sci.*, **92**, 3940 (1998).
6. E.W.Montroll, G.H.Weiss, *J.Math. Phys.*, **6**, 167 (1965).
7. V.V.Afanasiev, R.Z.Sagdeev, G.M.Zaslavsky, *Chaos* 1(2), 143 (1991).
8. V.V.Uchaikin, *Physica A* **255**, 65 (1998).
9. W.Feller, *Introduction to Probability Theory and Its Applications* (Vol. II, J.Wiley, New York, 1971).

10. S.G.Samko, A.A.Kilbas, O.I.Marichev, *Fractional Integrals and Derivatives – Theory and Applications* (Gordon and Breach, New York, 1993).

11. V.V.Uchaikin, V.M.Zolotarev, *Chance and Stability. Stable Distributions and their Applications* (VSP, Utrecht, The Netherlands, 1999).

12. V.M.Zolotarev, *One-dimensional Stable Distributions* (Amer. Math. Soc., Providence, R.I., 1986).

13. A.M. Mathai, R.K.Saxena, *The H-function with Applications in Statistics and Other Disciplines* (Wiley, New Delhi, 1978).

14. V.M.Zolotarev, V.V.Uchaikin, V.V.Saenko, *Journ. of Exper. and Theor. Physics*, **88**, 780 (1999).

15. V.V.Uchaikin, *Journ. of Exper. and Theor. Physics*, **88**, 1155 (1999).

16. J.-P.Bouchaud and A.Georges, *Phys. Rep.*, **195**, 127 (1990).